SQU Journal for Science, 2014, 19(1), 95-104

FCC, BCC and SC Lattices Derived from the Coxeter-Weyl groups and Quaternions

Nazife Özdeş Koca*, Mehmet Koca and Muna Al-Sawafi

*Department of Physics, College of Science, Sultan Qaboos University, P.O. Box: 36, PC 123, Al-Khod, Muscat, Sultanate of Oman. *E-mail: nazife@squ.edu.om.*

ABSTRACT: We construct the fcc (face centered cubic), bcc (body centered cubic) and sc (simple cubic) lattices as the root and the weight lattices of the affine extended Coxeter groups $W(A_3)$ and $W(B_3) \approx Aut(A_3)$. It is naturally expected that these rank-3 Coxeter-Weyl groups define the point tetrahedral symmetry and the octahedral symmetry of the cubic lattices which have extensive applications in materials science. The imaginary quaternionic units are used to represent the root systems of the rank-3 Coxeter-Dynkin diagrams which correspond to the generating vectors of the lattices of interest. The group elements are written explicitly in terms of pairs of quaternions which constitute the binary octahedral group. The constructions of the vertices of the Wigner-Seitz cells have been presented in terms of quaternionic imaginary units. This is a new approach which may link the lattice dynamics with quaternion physics. Orthogonal projections of the lattices onto the Coxeter plane represent the square and honeycomb lattices.

Keywords: Coxeter groups; Lattices; Quaternions.

شبكات المكعب البسيط (SC) والمكعب مركزي الجسم (BCC) والمكعب مركزي الوجه (FCC) المشتقة من مجموعات كوسيتر- ويل والكواتيرنيون

نظيفة كوجا، مهمت كوجا و منى الصوافية

ملخص : لقد تم بناء شبكات المكعب البسيط (SC) والمكعب مركزي الجسم (BCC) والمكعب مركزي الوجه (FCC) من الشبكة الأساسية والشبكة التثاقلية لمجموعات كوسيتر المترابطة والممتدة (affine extended Coxeter) $W(A_3)$ و $W(B_3) \approx Aut(A_3)$. إن مجموعات كوسيتر- ويل (Coxeter-Weyl) ذات المرتبة الثالثة تمتلك تناظر (تماثل) رباعي وثماني لشبكة المكعب والتي لديها تطبيقات واسعة في مجال علم المواد. إن وحدات العدد المركب التخيلي كواتيرنيون (quaternions) استخدمت لتمثل النظام الأساسي لمخططات كوسيتر-دينكن (Coxeter-Dynkin) ذو المرتبة الثالثة لإيجاد متجهات الشبكة. عناصر المجموعة كتبت بدلالة أزواج من كواتيرنيون تشكل المجموعة الثمانية الثنائية. كما تم تمثيل رؤوس (قمم) خلايا ويجنر-زيتز (Wigner-Seitz) بدلالة وحدات العدد المركب التخيلي كواتيرنيون (quaternions). وهذا النهج الجديد قد يربط بين ديناميكية الشبكة مع فيزياء الكواتيرنيون. الإسقاط العمودي للشبكة على سطح كوسيتر (Coxeter) يمثل شبكة المربع والشبكة السداسية (خلية النحل).

مفتاح الكلمات: مجموعات كوكستر، الشبيكة الفراغية و الرباعيات المركبة.

1. Introduction

The Lie groups based on the Coxeter-Weyl groups [1] have had a great impact in high energy physics, describing its Standard Model [2-4] and its extension to the Grand Unified theories [5-7]. The Coxeter-Weyl groups acting as discrete groups in the 3D Euclidean space generate certain orbits [8-9] which describe the molecular structures [10] and viral symmetries [11-12]. Higher dimensional lattices described by the affine extension of the Coxeter-Weyl groups can be used to describe the quasicrystal structures when projected into lower dimensions [13-16]. The rank-3 Coxeter-Weyl groups $W(A_3)$ and $W(B_3) \approx Aut(A_3)$ define the point tetrahedral and octahedral symmetries of the cubic lattices which have an enormous number of applications in materials science. In this paper we explicitly show that the root lattice and the weight lattice of the affine Coxeter group $W_a(A_3)$ describe the fcc and bcc lattices respectively. We point out that there is a natural correspondence between the octahedral symmetry of the fcc and bcc lattices and the binary octahedral group of quaternions. The paper is organized as follows.

In Section 2 we explore how the honeycomb lattice and the square lattice in two dimensions are respectively described by the affine extensions of the Coxeter-Weyl groups $W(A_2)$ and $W(B_2)$ respectively. Section 3 is devoted to the construction of the Coxeter-Weyl group $W(A_3)$ and its extension $Aut(A_3)$ by Dynkin diagram symmetry in terms of quaternions. We explicitly display how those polyhedra possessing tetrahedral symmetry can be constructed as the orbits of the group $W(A_3)$ and prove that the root lattice and the weight lattice describe the fcc and the bcc lattices respectively. In Section 4 we point out that the regular polyhedra can be obtained as the orbits of the Coxeter-Weyl group $W(B_3)$ and furthermore we demonstrate that its affine extension $W_a(B_3)$ describes the sc and the bcc lattices as the root and the weight lattices of B_3 expressed in terms of quaternions. In Section 5 we study the orthogonal projections of A_3 and B_3 lattices onto the Coxeter plane, displaying respectively the square and hexagonal lattices and emphasize the importance of the dihedral subgroups of the Coxeter-Weyl groups in projection techniques. Some conclusive remarks will be presented in Section 6 regarding the applications of the quaternionic constructions of the 3D lattices.

2. Construction of the honeycomb and square lattices as the affine Coxeter-Weyl groups W$_a$ (A_2) and W$_a$ (B_2)

The Coxeter-Weyl groups are generated by reflections with respect to some hyperplanes represented by vectors (also called roots in the literature of Lie algebras). If $r_1, r_2, ..., r_n$ represent the reflection generators, then the presentation of the Coxeter-Weyl group $W(G)$ is given by

$$W(G) = \langle r_1, r_2, ..., r_n \,|\, (r_i\, r_j)^{m_{ij}} = 1 \rangle \tag{1}$$

where m_{ij} is an integer label with $m_{ii} = 1,\ m_{ij} = 2, 3, 4$ and 6 for $i \neq j$ representing respectively no line, one line, two lines (or label 4) and three lines (or label 6) between the nodes of the Coxeter-Dynkin diagrams which determine the crystallographic groups. In case m_{ij} takes other positive integer values they correspond to non-crystallographic Coxeter groups which are out of the scope of this work. The Coxeter-Dynkin diagrams representing the groups $W(A_2)$ and $W(B_2)$ that we will study in this section are given in Figure 1.

Figure 1. The Coxeter-Dynkin diagrams (a) for A_2 and (b) for B_2.

The vectors α_1 and α_2 (hereafter called 'roots') orthogonal to the planes with respect to which the reflection generators reflect an arbitrary vector Λ as

$$r_i \Lambda = \Lambda - \frac{2(\Lambda, \alpha_i)}{(\alpha_i, \alpha_i)} \alpha_i, \ i = 1, 2. \tag{2}$$

The Cartan matrix C with the matrix elements $C_{ij} = \frac{2(\alpha_i, \alpha_j)}{(\alpha_j, \alpha_j)}$ and the metric G defined by matrix elements $G_{ij} = (C^{-1})_{ij} \frac{(\alpha_j, \alpha_j)}{2}$ are important for the description of the Coxeter-Weyl groups and the corresponding lattices. The Cartan matrix and the matrix G represent the Gram matrices of the direct lattice and the reciprocal lattice respectively [17]. We take the roots α_i as the generating vectors of the direct lattice. The weights ω_i spanning the dual space and satisfying the scalar product

$(\omega_i, \omega_j) = G_{ij}$ and $(\omega_i, \breve{\alpha}_j) = \delta_{ij}$ with $\breve{\alpha}_j \equiv \frac{2\alpha_j}{(\alpha_j, \alpha_j)}$ correspond to the generating vectors of the reciprocal lattice. Now we discuss the lattices associated with each Coxeter-Weyl group.

2.1 The lattice determined by the affine group W$_a$(A_2)

The Cartan matrix C and the metric G are given as follows

$$C = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \quad G = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}. \tag{3}$$

The plot of the polygons (triangle or hexagon) described by the orbits of the group $W(A_2)$ will be given in orthonormal basis which can be obtained by using the eigenvectors of the Cartan matrix [18]

$$\hat{x}_1 = \frac{1}{\sqrt{2}}(\alpha_1 + \alpha_2),\ \hat{x}_2 = \frac{1}{\sqrt{6}}(\alpha_1 - \alpha_2) \tag{4}$$

and in the orthonormal basis the roots read as

$$\alpha_1 = (\frac{1}{\sqrt{2}}, \sqrt{\frac{3}{2}}),\ \alpha_2 = (\frac{1}{\sqrt{2}}, -\sqrt{\frac{3}{2}}). \tag{5}$$

The group generators act on the roots as:
$r_1\alpha_1 = -\alpha_1, r_1\alpha_2 = \alpha_2 + \alpha_1, r_2\alpha_1 = \alpha_1 + \alpha_2, r_2\alpha_2 = -\alpha_2$ which generate the group $W(A_2)$ of order 6, which is isomorphic to the dihedral group D_3. Including the Dynkin diagram symmetry which implies $\gamma : \alpha_1 \leftrightarrow \alpha_2$, the generators generate a group of order 12, which is isomorphic to the dihedral group D_6. The matrix representations of the generators in the root space can be written as

$$r_1 = \begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix},\ r_2 = \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix},\ \gamma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{6}$$

The affine Coxeter group $W_a(A_2)$ includes another generator r_0 which reflects the vectors with respect to a plane bisecting the vector $\alpha_1 + \alpha_2$. This corresponds to a translation on an arbitrary vector Λ, as $\Lambda \to \Lambda + (\alpha_1 + \alpha_2)$. The repeated applications of the generators will generate the root lattice A_2, where an arbitrary lattice vector is given by $p = b_1\alpha_1 + b_2\alpha_2$, with $b_1, b_2 \in \mathbb{Z}$ (the set of integers). The root system consisting of the vectors $\pm\alpha_1, \pm\alpha_2, (\pm\alpha_1 \pm \alpha_2)$ determines the primitive cell of the direct lattice which is an hexagon. The whole lattice is the infinite set of hexagons as shown in Figure 2. It is interesting that the honeycomb lattice does in fact exist as graphene made of carbon atoms [19].

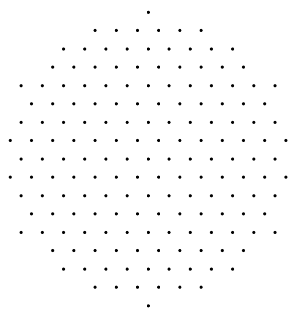

Figure 2. The honeycomb lattice.

The weight vectors can be determined from the relation $\omega_i = \sum_{j=1}^{2} G_{ij}\alpha_j$ where the reciprocal lattice A_2^* (weight lattice) vectors are given by $q = a_1\omega_1 + a_2\omega_2 \equiv (a_1, a_2)$ with $a_1, a_2 \in \mathbb{Z}$. We will define an orbit in the dual space (reciprocal space) as $W(A_2)(a_1, a_2) \equiv (a_1, a_2)_{A_2}$ which represents an isogonal hexagon with two edge lengths in general. When we have $a_1 = a_2$, the orbit is a regular hexagon $(1,1)_{A_2}$ determined by the root system which is invariant under the group $Aut(A_2) \approx W(A_2):C_2$ generated by the matrices in (6). The orbits $(a_1, 0)_{A_2}$ and $(0, a_2)_{A_2}$ represent triangles. The union of the orbits $(1,0)_{A_2} \oplus (0,1)_{A_2}$, each representing an equilateral triangle, constitutes another hexagon dual to the hexagon $(1,1)_{A_2}$ and describes the primitive cell of the weight lattice. Since both the root lattice and the weight lattice are made of hexagons they can be transformed to each other by a change of scale and the lattice point symmetry. Note that the hexagon described by two triangles is invariant under the group $Aut(A_2)$ which involves the Dynkin diagram symmetry.

We assume that the reader is familiar with the concept of nearest neighbor region which is called the Wigner-Seitz cell or Brillouin zone by the crystallographers, but is also known as the Voronoi cell or Drichlet region by mathematicians. The Wigner-Seitz cell of the root lattice A_2 is the cell $(1,0)_{A_2} \oplus (0,1)_{A_2}$ which can be determined from its primitive cell (see Figure 3). The Wigner-Seitz cell $(1,0)_{A_2} \oplus (0,1)_{A_2}$ is a scaled copy of the dual of the primitive cell $(1,1)_{A_2}$ after a 30^0 rotation. It is obvious that the primitive cell of the weight lattice is the hexagon $(1,0)_{A_2} \oplus (0,1)_{A_2}$.

It can be shown that the Wigner-Seitz cell of the weight lattice is the orbit $\frac{1}{3}(1,1)_{A_2}$, which is a scaled copy of the root polyhedron (hexagon in this case) by the Coxeter number 3 of the group $W(A_2)$. We will see that this is a general property of the A_n series of the Coxeter-Weyl groups.

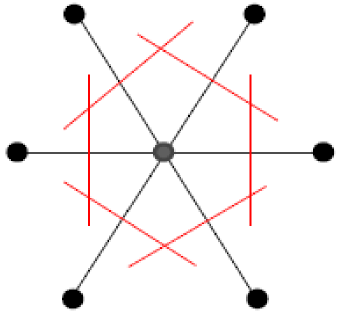

Figure 3. The Wigner-Seitz cell $(1,0)_{A_2} \oplus (0,1)_{A_2}$ inscribed in the primitive cell of the root lattice.

2.2 The lattice determined by the affine group W$_a$ (B_2)

The roots of B_2 consist of long and short roots; in a particular orthonormal system with $(l_i, l_j) = \delta_{ij}$, the simple roots can be written as $\alpha_1 = l_1 - l_2, \alpha_2 = l_2$. The Cartan matrix, its inverse and the matrix G are given by

$$C = \begin{pmatrix} 2 & -2 \\ -1 & 2 \end{pmatrix},\ C^{-1} = \begin{pmatrix} 1 & 1 \\ \frac{1}{2} & 1 \end{pmatrix},\ G = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{7}$$

The group generators r_1 and r_2 act in the root space as

$$r_1\alpha_1 = -\alpha_1, r_1\alpha_2 = \alpha_1 + \alpha_2, r_2\alpha_1 = \alpha_1 + 2\alpha_2, r_2\alpha_2 = -\alpha_2 \tag{8}$$

which can be represented by the matrices

$$r_1 = \begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix},\ r_2 = \begin{pmatrix} 1 & 2 \\ 0 & -1 \end{pmatrix}. \tag{9}$$

They generate the dihedral group D_4 of order 8, which is the symmetry of the square. The root system consists of two orbits $\{\pm\alpha_2,\ \pm(\alpha_1+\alpha_2)\}$ and $\{\pm\alpha_1,\ \pm(\alpha_1+2\alpha_2)\}$ which can also be written in the orthonormal basis as $\{\pm l_1,\ \pm l_2\}$ and $\{\pm l_1 \pm l_2\}$, corresponding to the centers of the edges and the vertices of a square respectively. It is clear that the root lattice is generated by the short roots of B_2.The primitive cell is the square represented by the vectors $\{\pm l_1,\ \pm l_2\}$. The translation generator is obtained as the addition of the highest short root $\alpha_1+\alpha_2 = l_1$ to any vector. Therefore the root lattice is represented either by the vectors $b_1\alpha_1+b_2\alpha_2;\ b_1, b_2 \in \mathbb{Z}$ or, equivalently, by $m_l l_1+m_2 l_2;\ \ m_1,\ m_2 \in \mathbb{Z}$. Then the Wigner–Seitz cell is a square with the vertices $(0,1)_{B_2} = \{\pm\frac{1}{2}l_1 \pm \frac{1}{2}l_2\}$ as shown in Figure 4.

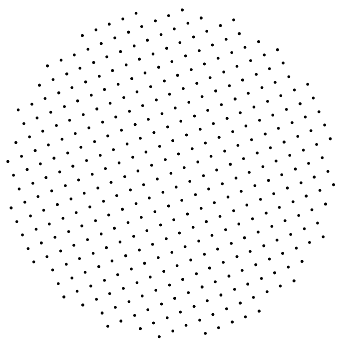

Figure 4. The square lattice as the root lattice of B_2.

The weight lattice is represented by the vectors $a_1\omega_1+a_2\omega_2,\ \ a_1,\ a_2 \in \mathbb{Z}$. Then the lattice vectors in the orthonormal basis will be $m_l l_1+m_2 l_2;\ \ 2m_1,\ 2m_2 \in \mathbb{Z}$ so that it involves the union of the sets with m_1 and m_2 are either both integers or both half integers. This indicates also that the root lattice is a sublattice of the weight lattice. Since the weight lattice and the root lattice are equivalent to each other up to a scale transformation and a rotation by 45^0, it suffices to talk about the root lattice only.

3. Construction of the fcc and the bcc lattices as the affine Coxeter-Weyl group $W_a(A_3)$

A brief introduction is necessary for those readers not familiar with the quaternions. The quaternions are the extension of the complex number system discovered by Hamilton in 1853 [20] with three imaginary units i, j, k satisfying the well-known relations

$$i^2 = j^2 = k^2 = -1, \;\; ijk = -1.$$

In what follows we will use a different notation for the quaternionic units $i \to e_1, j \to e_2, k \to e_3$. Let $q = q_0 + q_i e_i$, $(i = 1, 2, 3)$ be a real unit quaternion with its conjugate defined by $\bar{q} = q_0 - q_i e_i$ and its norm $q\bar{q} = \bar{q}q = 1$.
The quaternionic imaginary units now satisfy the relations

$$e_i e_j = -\delta_{ij} + \varepsilon_{ijk} e_k, \;\; (i, j, k = 1,2,3) \tag{10}$$

where δ_{ij} and ε_{ijk} are the Kronecker and Levi-Civita symbols, and summation over the repeated indices is understood. The unit quaternions form a group isomorphic to the special unitary group $SU(2)$. With the definition of the scalar product

$$(p,q) = \frac{1}{2}(\bar{p}q + \bar{q}p) = \frac{1}{2}(p\bar{q} + q\bar{p}) \tag{11}$$

quaternions generate the four-dimensional Euclidean space and the unit quaternions $1, e_1, e_2$ and e_3 form an orthonormal basis. From now on it is understood that a quaternion is a 4D-Euclidean vector. The Coxeter-Dynkin diagram of A_3 with the quaternionic simple roots is given in Figure 5.

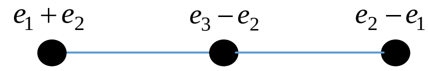

Figure 5. The Coxeter diagram A_3 with quaternionic simple roots.

An arbitrary quaternion Λ when reflected by the operator r with respect to the hyperplane orthogonal to quaternion α is given in terms of quaternion multiplication [21] as

$$r\Lambda = -\frac{\alpha}{\sqrt{2}}\bar{\Lambda}\frac{\alpha}{\sqrt{2}} \equiv [\frac{\alpha}{\sqrt{2}}, -\frac{\alpha}{\sqrt{2}}]^*\Lambda \,. \tag{12}$$

The bracket on the right of the equation (12) is self explanatory and should not be confused with the commutator notation. The Cartan matrix of the Coxeter-Dynkin diagram A_3 and its inverse matrix are given respectively by the matrices

$$C = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}, \;\; C^{-1} = \frac{1}{4}\begin{bmatrix} 3 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 3 \end{bmatrix}. \tag{13}$$

The generators of the Coxeter group $W(A_3)$ are then given in the notation of (12) by

$$r_1 = [\frac{1}{\sqrt{2}}(e_1 + e_2), -\frac{1}{\sqrt{2}}(e_1 + e_2)]^*,$$

$$r_2 = [\frac{1}{\sqrt{2}}(e_3 - e_2), -\frac{1}{\sqrt{2}}(e_3 - e_2)]^*, \; r_3 = [\frac{1}{\sqrt{2}}(e_2 - e_1), -\frac{1}{\sqrt{2}}(e_2 - e_1)]^*. \tag{14}$$

The reflection generators operate on the quaternionic imaginary units as follows:

$$r_1 : e_1 \leftrightarrow -e_2, \; e_3 \to e_3; \;\; r_2 : e_1 \to e_1, \; e_2 \leftrightarrow e_3; \; r_3 : e_1 \leftrightarrow e_2, \; e_3 \to e_3.$$

They generate the Coxeter group $W(A_3)$ of order 24 isomorphic to the tetrahedral group, the elements of which can be written compactly by the set

$$W(A_3) = \{[p, \bar{p}] \oplus [t, \bar{t}]^*\}, \; p \in T, \; t \in T'. \tag{15}$$

Here T and T' are the sets of quaternions

$$T = \{ \pm 1,\ \pm e_1,\ \pm e_2,\ \pm e_3,\ \frac{1}{2}(\pm 1 \pm e_1 \pm e_2 \pm e_3)\},$$

$$T' = \{\tfrac{1}{\sqrt{2}}(\pm 1 \pm e_1), \tfrac{1}{\sqrt{2}}(\pm e_2 \pm e_3), \tfrac{1}{\sqrt{2}}(\pm 1 \pm e_2), \tfrac{1}{\sqrt{2}}(\pm e_3 \pm e_1), \tfrac{1}{\sqrt{2}}(\pm 1 \pm e_3), \tfrac{1}{\sqrt{2}}(\pm e_1 \pm e_2)\} \quad (16)$$

where T represents the binary tetrahedral group of order 24, and the union of the set $O = T \oplus T'$ represents the binary octahedral group [22] of order 48 . When the simple roots are chosen $\alpha_1 = e_1 + e_2, \alpha_2 = e_3 - e_2, \alpha_3 = e_2 - e_1$ as in the Figure 5 then the weight vectors are determined from (13) as

$$\omega_1 \equiv (1,0,0) = \frac{1}{2}(e_1 + e_2 + e_3), \quad \omega_2 \equiv (0,1,0) = e_3, \quad \omega_3 \equiv (0,0,1) = \frac{1}{2}(-e_1 + e_2 + e_3)\,. \quad (17)$$

The orbits generated by these vectors would lead to the set of vectors

$$\begin{aligned}
(1,0,0)_{A_3} &= \{\frac{1}{2}(e_1 + e_2 + e_3), \frac{1}{2}(e_1 - e_2 - e_3), \frac{1}{2}(-e_1 - e_2 + e_3), \frac{1}{2}(-e_1 + e_2 - e_3)\},\\
(0,1,0)_{A_3} &= \{\pm e_1,\ \pm e_2,\ \pm e_3\}, \qquad (18)\\
(0,0,1)_{A_3} &= \{\frac{1}{2}(-e_1 - e_2 - e_3), \frac{1}{2}(-e_1 + e_2 + e_3), \frac{1}{2}(e_1 + e_2 - e_3), \frac{1}{2}(e_1 - e_2 + e_3)\}.
\end{aligned}$$

They respectively represent the vertices of a tetrahedron, an octahedron and another tetrahedron. The orbits $(1,0,0)_{A_3}$ and $(0,0,1)_{A_3}$ together represent the vertices of a cube. Therefore the symmetry of the union of the orbits $(1,0,0)_{A_3} \oplus (0,0,1)_{A_3}$ requires the Dynkin diagram symmetry $\gamma = [e_1, -e_1]^*$ which extends the Coxeter group $W(A_3)$ to the octahedral group $Aut(A_3) \approx W(A_3):C_2$ whose quaternionic representation is given by

$$Aut(A_3) = \{[T,\bar{T}] \oplus [T',\bar{T}']^* \oplus [T,\bar{T}]^* \oplus [T',\bar{T}']\}\,. \quad (19)$$

Note that from now on we are using the group notation instead of (15), but with the same meaning. It can be proved that the Coxeter-Weyl group $W(A_3)$ given by (15) is isomorphic to tetrahedral group $W(A_3) \approx T_d \approx S_4$ where the notation T_d is used by crystallographers and S_4 represents the symmetric group of four objects which permutes the vertices of a tetrahedron. To understand this better, let us denote the vertices of the tetrahedron by letters;

$$A = \frac{1}{2}(e_1 + e_2 + e_3), B = \frac{1}{2}(e_1 - e_2 - e_3), C = \frac{1}{2}(-e_1 - e_2 + e_3), D = \frac{1}{2}(-e_1 + e_2 - e_3).$$

It is clear now that the reflection generators can be written in the permutation notations

$$r_1 = \begin{pmatrix} A & B & C & D \\ C & B & A & D \end{pmatrix},\ r_2 = \begin{pmatrix} A & B & C & D \\ A & B & D & C \end{pmatrix},\ r_3 = \begin{pmatrix} A & B & C & D \\ A & D & C & B \end{pmatrix}. \quad (20)$$

In this notation they represent the generators of the group S_4, permuting the four letters. To see a few examples, note that $r_1 r_2$ fixes *B* but permutes *ACD*. Similarly $r_2 r_3$ leaves *A* invariant but permutes *BDC*. The Coxeter element $r_1 r_2 r_3$ permutes all four letters in the order *ACDB*. The group $Aut(A_3)$ has three maximal subgroups, each is of order 24.

a) The usual one is the $W(A_3) = \{[T,\bar{T}] \oplus [T',\bar{T}']^*\}$ tetrahedral group derived from the Coxeter-Dynkin diagram and it is the symmetry of a tetrahedron as we have seen.

b) The group $W(A_3)/C_2 = \{[T,\bar{T}] \oplus [T',\bar{T}']\}$ is the proper rotational subgroup of the octahedral group $Aut(A_3)$. In another paper [23] we have proved that it is the symmetry of the snub cube, a chiral polyhedron, and one can construct the vertices of the snub cube by the action of the group on a vector.

The group $T_h \approx A_4 \times C_2 = \{[T,\bar{T}] \oplus [T,\bar{T}]^*\}$ is the pyritohedral group representing symmetry of a pyritohedron, an irregular dodecahedron with irregular pentagonal faces which occurs in pyrites. For the interested reader we give here the matrix representations of the generators of the group $Aut(A_3)$ acting on the quaternionic imaginary units.

$$r_1=\begin{bmatrix}0&-1&0\\-1&0&0\\0&0&1\end{bmatrix},\ r_2=\begin{bmatrix}1&0&0\\0&0&1\\0&1&0\end{bmatrix},\ r_3=\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix},\ \gamma=\begin{bmatrix}-1&0&0\\0&1&0\\0&0&1\end{bmatrix}\tag{21}$$

3.1 The fcc lattice as the root lattice of A_3

The group generators of the affine $W_a(A_3)$ are the three reflection generators r_1, r_2, r_3 and r_0, where r_0 acts like a translation by the highest root $\alpha_H=\alpha_1+\alpha_2+\alpha_3=e_2+e_3$, that is, $r_0\Lambda=\Lambda+\alpha_H$. A general vector of the root lattice is then given by $p=b_1\alpha_1+b_2\alpha_2+b_3\alpha_3;\ b_1,b_2,b_3\in\mathbb{Z}$ which can be written in terms of quaternions as

$$p=m_1e_1+m_2e_2+m_3e_3;\ m_1,m_2,m_3\in\mathbb{Z}.\tag{22}$$

The root system of A_3 is the orbit $(1,0,1)_{A_3}=\{\pm e_1\pm e_2,\pm e_2\pm e_3,\pm e_3\pm e_1\}$ consisting of 12 quaternions representing the centers of the edges of a cube. Including the orbit $(0,0,0)_{A_3}$ which corresponds to the origin, the root system represents the "non-conventional" face centered cubic cell [24]. It is easy to prove that the Wigner-Seitz cell of the fcc lattice is the Catalan solid, the rhombic dodecahedron, dual to the Archimedean solid cuboctahedron determined by the root system of A_3. The vertices of the rhombic dodecahedron which constitutes the Wigner-Seitz cell can then be written as the union of the orbits $(1,0,0)_{A_3}\oplus(0,1,0)_{A_3}\oplus(0,0,1)_{A_3}$ whose quaternionic vertices are given in (18). The rhombic dodecahedron represented by the set of vertices is depicted in Figure 6.

The centers of the faces of the rhombic dodecahedron are the vertices given by $\frac{1}{2}(1,0,1)_{A_3}=\frac{1}{2}\{\pm e_1\pm e_2,\pm e_2\pm e_3,\pm e_3\pm e_1\}$. Note that the rhombic dodecahedron tiles the 3D Euclidean space, however, it is not vertex transitive under the group $Aut(A_3)$, but rather face transitive.

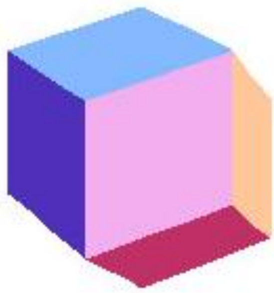

Figure 6. The rhombic dodecahedron, Wigner –Seitz cell of the fcc lattice.

3.2 The bcc lattice as the weight lattice of A_3

The weight lattice A_3^* is generated by three weight vectors $\omega_1\equiv(1,0,0),\quad \omega_2\equiv(0,1,0),\quad \omega_3\equiv(0,0,1)$. A general vector of the lattice is given by $q=a_1\omega_1+a_2\omega_2+a_3\omega_3,\ a_1,a_2,a_3\in\mathbb{Z}$. In terms of quaternions, a weight lattice vector consists of the linear combinations of the quaternionic units; the coefficients of the unit vectors are either all integers or half integers. Recall that the root lattice consists of the quaternions obtained as the linear coefficients of the quaternionic imaginary units with integer coefficients only. We note that the orbits $(1,0,0)_{A_3}\oplus(0,0,0)_{A_3}\oplus(0,0,1)_{A_3}$ form the body centered cubic cell where the origin represents the central lattice point. One can easily prove that the nearest lattice points to the origin are the orbits $(1,0,0)_{A_3}\oplus(0,1,0)_{A_3}\oplus(0,0,1)_{A_3}$. From (18) we deduce that the distance to the lattice points represented by the vertices of the square $(1,0,0)_{A_3}\oplus 0,0,1)_{A_3}$ is $\frac{\sqrt{3}}{2}\approx 0.866$, but the next nearest points are on the orbit $(0,1,0)_{A_3}$ at a distance 1. As usual, the walls of the Wigner-Seitz cell bisect the lines joining these nearest points to the origin. It is easy to show that the intersections of these planes determine the vertices of the Wigner-Seitz cell as the orbit $\frac{1}{4}(1,1,1)_{A_3}$, which is a truncated octahedron as shown in Figure 7, and the vertices of which are given by

$$\frac{1}{4}(1,1,1)_{A_3}=\frac{1}{4}\{\pm e_1\pm 2e_2,\pm e_2\pm 2e_3,\pm e_3\pm 2e_1,\pm 2e_1\pm e_2,\pm 2e_2\pm e_3,\pm 2e_3\pm e_1\}.\tag{23}$$

Figure 7. Truncated octahedron.

4. Construction of the sc and the bcc lattices as the affine Coxeter-Weyl groups $W_a(B_3)$

The Coxeter-Dynkin diagram of B_3 leading to the octahedral group $W(B_3) \approx O_h$ is shown in Figure 8.

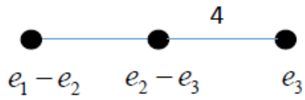

Figure 8. The Coxeter-Dynkin diagram of B_3 with quaternionic simple roots.

The Cartan matrix of the Coxeter-Dynkin diagram of B_3 and its inverse matrix are given by

$$C = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -2 \\ 0 & -1 & 2 \end{bmatrix}, \; C^{-1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2 \\ \frac{1}{2} & 1 & \frac{3}{2} \end{bmatrix}, \; G = \begin{bmatrix} 1 & 1 & \frac{1}{2} \\ 1 & 2 & 1 \\ \frac{1}{2} & 1 & \frac{3}{4} \end{bmatrix}. \tag{24}$$

The generators,

$$r_1 = [\frac{1}{\sqrt{2}}(e_1 - e_2), -\frac{1}{\sqrt{2}}(e_1 - e_2)]^* ; r_2 = [\frac{1}{\sqrt{2}}(e_2 - e_3), -\frac{1}{\sqrt{2}}(e_2 - e_3)]^* ; \; r_3 = [e_3, -e_3]^* \tag{25}$$

generate the octahedral group which can be written as

$$W(B_3) \approx Aut(A_3) \approx S_4 \times C_2 = \{[p,\bar{p}] \oplus [p,\bar{p}]^* \oplus [t,\bar{t}] \oplus [t,\bar{t}]^*\}, \; p \in T, t \in T'. \tag{26}$$

where the shorthand notation $W(B_3) = \{[T,\bar{T}] \oplus [T,\bar{T}]^* \oplus [T',\bar{T}'] \oplus [T',\bar{T}']^*\}$ is given in (19). The weight vectors ω_1, ω_2 and ω_3 are determined from the simple roots $\alpha_1 = e_1 - e_2, \alpha_2 = e_2 - e_3, \alpha_3 = e_3$ as

$$\omega_1 = e_3, \omega_2 = e_1 + e_2, \omega_3 = \frac{1}{2}(\pm e_1 \pm e_2 \pm e_3). \tag{27}$$

The orbits $(1,0,0)_{B_3}, (0,1,0)_{B_3}$, and $(0,0,1)_{B_3}$ represent an octahedron, a cuboctahedron and a cube respectively. Here the orbit $(1,1,0)_{B_3}$ represents the truncated octahedron which is obtained as the orbit $(1,1,1)_{A_3}$ under the group $W(A_3)$. Note that B_3 consists of long roots and short roots of norms $\sqrt{2}$ and 1 respectively. The octahedral group $W(B_3) \approx O_h$ in (26) generates a root system consisting of the roots

$$(1,0,0)_{B_3} \oplus (0,1,0)_{B_3} = \{\pm e_1, \pm e_2, \pm e_3\} \oplus \{\pm e_1 \pm e_2, \pm e_2 \pm e_3, \pm e_3 \pm e_1\}. \tag{28}$$

It is clear from (28) that they constitute two different orbits; however the second set is merely a linear combination of the first set of vectors.

By the affine extension of B_3 we note that the quaternionic highest root is $\alpha_H = e_1 + e_2$. Therefore the generator r_0 corresponding to the highest root $\alpha_H = e_1 + e_2$ leads to a translation $r_0\Lambda = \Lambda + e_1 + e_2$. This represents a reflection of the origin with respect to the plane bisecting the vector ω_2 at the point $\frac{\omega_2}{2}$. A general root lattice vector is then given by $p = b_1\alpha_1 + b_2\alpha_2 + b_3\alpha_3$, with $b_1, b_2, b_3 \in \mathbb{Z}$.

4.1 The sc lattice as the root lattice of B_3

The root lattice is generated by the short roots e_1, e_2, e_3 of B_3 and a general root lattice vector is given in terms of quaternionic units as $p = m_1 e_1 + m_2 e_2 + m_3 e_3;\ m_1, m_2, m_3 \in \mathbb{Z}$. Including the origin the simple cube has the vertices

$$0,\ e_1,\ e_2,\ e_3,\ e_1+e_2,\ e_2+e_3,\ e_3+e_1,\ e_1+e_2+e_3. \tag{29}$$

The reciprocal lattice has the same generator vectors $e_1,\ e_2,\ e_3$. The Wigner-Seitz cell can be determined around the origin by bisecting the lines joining the origin to the vertices $\pm e_1, \pm e_2, \pm e_3$. Intersecting planes determine the vertices of the Wigner-Seitz cell which represents the cube given by the orbit

$$(0,0,1)_{B_3} = \frac{1}{2}(\pm e_1 \pm e_2 \pm e_3). \tag{30}$$

4.2 The bcc lattice as the weight lattice of B_3

The weight lattice is exactly the same lattice as determined by the weight lattice A_3^*, since the weight vectors will be the linear combinations of the quaternionic imaginary units with either integer coefficients or half integer coefficients. Here the nearest neighbors of the origin are the vectors $\frac{1}{2}(\pm e_1 \pm e_2 \pm e_3)$ and $\{\pm e_1,\ \pm e_2,\ \pm e_3\}$. As we have seen in the case of A_3^*, the Wigner-Seitz cell is the truncated octahedron whose vertices are determined as the orbit $\frac{1}{4}(1,1,0)_{B_3}$.

5. Projections of the A_3 and B_3 lattices onto their Coxeter planes

Projection of higher dimensional lattices to lower dimensional spaces is an interesting technique in the description of quasicrystallography. In reference [18] we proposed that in the projection technique the Coxeter number and the Coxeter integers play important roles. We here describe the technique in applying it to A_3 and B_3 lattices although the result is not a quasi crystal. Every Coxeter group has a maximal dihedral subgroup of order $2h$ where h is the Coxeter number. It goes as follows: partition the simple roots into two sets of roots so that each set consists of orthogonal roots. In the case of A_3 and B_3 these sets are $\{\alpha_1,\ \alpha_3\}$ and α_2. We now consider the case of A_3 where we define the Coxeter plane determined by the vectors given by

$$\beta_1 = \frac{1}{\sqrt{2}}(\alpha_1 + \alpha_3\} = \sqrt{2}\mathrm{e}_2\ ,\ \beta_2 = \alpha_2 = e_2 - e_3 \tag{31}$$

which is orthogonal to the vector $\beta_3 = \frac{1}{\sqrt{2}}(\alpha_1 - \alpha_3\} = \sqrt{2}\mathrm{e}_1$. We now define the generators $R_1 = r_1 r_3$ and $R_2 = r_2$ which satisfy the relation $(R_1 R_2)^4 = 1$. Orthogonal projection will be made onto the Coxeter plane determined by the vectors β_1 and β_2 in which R_1 and R_2 act as reflection generators. R_1 and R_2 do in fact generate the dihedral subgroup D_4 of A_3 of order 8. The orthogonal set of vectors in the Coxeter plane can be taken as the quaternionic unit vectors e_2 and e_3. Let us recall that the root lattice vectors are given by $p = m_1 e_1 + m_2 e_2 + m_3 e_3;\ m_1, m_2, m_3 \in \mathbb{Z}$. The orthogonal projection of the A_3 lattice means one takes only the set of vectors $m_2 e_2 + m_3 e_3;\ m_2, m_3 \in \mathbb{Z}$ which constitutes a square lattice, or in other words, the root lattice of the Coxeter-Weyl group B_2 as shown in Figure 4. Projection of the weight lattice onto the Coxeter plane also includes the set of quaternions e_2 and e_3 with half integer coefficients as shown in Figure 4.

For the orthogonal projection of the lattice B_3, we follow the same technique; however the group generated by the generators R_1 and R_2 is the dihedral group D_6 of order 12 since $(R_1 R_2)^6 = 1$. Here the Coxeter plane is determined by the vectors $\beta_1 = \frac{1}{\sqrt{3}}(e_1 - e_2 + 2e_3)$ and $\beta_2 = e_2 - e_3$. Since the angle between them is 150^0, the reflection generators generate the dihedral group D_6 of order 12. This is the symmetry of a hexagon. The third vector $\beta_3 = \frac{1}{\sqrt{3}}(-e_1 + e_2 + e_3)$ is orthogonal to the Coxeter plane. The projection of the B_3 lattice onto the Coxeter plane will lead to a honeycomb lattice as shown in Figure 2.

6. Conclusion

The crystallographic Coxeter groups, in other words, the Coxeter-Weyl groups, are the skeleton of the Lie groups which may have many applications in quasicrystallography. We have shown in this paper that the Coxeter-Weyl groups acting in 2D and 3D directly describe the square, hexagonal, sc, fcc and bcc lattices. The advantage here is that they can be associated with some finite subgroups of quaternions and the vertices can be represented by quaternionic imaginary units. The symmetries of all these lattices have been explicitly demonstrated. This is a novel aspect of the quaternionic lattices in which not only the lattice vectors but also the group elements are represented by the quaternions. Since the quaternions can be used to describe the spin $\frac{1}{2}$ states of electrons or some atoms we anticipate that the lattice structures in 2D and/or 3D with explicit spin dependence can be described by the quaternionic lattice structures. Another interesting aspect of this work is that we have developed an orthogonal projection technique of the A_3 and B_3 lattices leading to the square and the honeycomb lattices respectively. It is an interesting observation that, if one views the 3D lattices from the Coxeter plane, one may observe the square or honeycomb lattice behaviors in the A_3 and B_3 lattices respectively.

References

1. Coxeter, H.S.M. and Moser, W.O.J. *Generators and Relations for Discrete Groups* Springer-Verlag, 1965.
2. Weinberg, S. A Model of Leptons. *Phys. Rev. Lett*., 1967, **19**, 1264-1266.
3. Salam, A. Elementary Particle Theory: Relativistic Groups and Analyticity. *Eighth Nobel Symposium, Stockholm* (Ed. Svartholm, N.), 1968, 367-377.
4. Fritzsch, H., Gell-Mann, M. and Leutwyler, H. Advantages of the colour octet gluon picture. *Phys. Lett.B*, 1973, **47**, 365-368.
5. Georgi, H. and Glashow, S. Unity of all elementary-particle forces. *Phys. Rev. Lett*., 1974, **32**, 438-441.
6. Fritzsch, H. and Minkowski, P. Unified interactions of leptons and hadrons. *Ann. Phys.*, 1975, **93**, 193-266.
7. Gürsey, F., Ramond, P. and Sikivie, P. A universal gauge theory model based on E6. *Phys. Lett.B*, 1976, **60**, 177-186.
8. Koca, M., Koc, R. and Al-Ajmi, M. Polyhedra obtained from Coxeter groups and quaternions. *J. Math. Phys*., 2007, **48**, 113514-113527.
9. Koca, M., Koca, N.O. and Koc, R. Catalan solids derived from 3D-root system. *J. Math. Phys.*, 2010, **51**, 043501-043513.
10. Cotton, F.S., Wilkinson, G., Murillo, C.A. and Bochmann, M. *Advanced Inorganic Chemistry* (6th Edition) Wiley-Inter science, New York, 1999.
11. Caspar, D.L.D. and Klug, A. Physical Principles in Construction of Regular Viruses. *Cold Spring Harbor Symp. Quant. Biol*., 1962, **27**, 1-24.
12. Twarock, R. A Mathematical Physicist's approach to the structure and assembly of viruses. *Phil. Trans. R. Soc. A*, 2006, **364**, 3357-3374.
13. Katz, A. and Duneau, M. Quasiperiodic patterns and icosahedral symmetry. *J. Phys. France*, 1986, **47**, 181-196.
14. Elser, V. The diffraction pattern of projected structures. *Acta Cryst. A*, 1986, **42**, 36-43.
15. Baake, M., Joseph, D., Kramer, P. and Schlottmann, M. Root lattices and quasicrystals. *J. Phys.* ***.*** *Math.and Gen. A*, 1990, **23**, L1037-L1041.
16. Baake, M., Kramer, P., Schlottmann, M. and Zeidler, D. Planar patterns with fivefold symmetry as sections of periodic structures in 4-space. *Int. J. Mod. Phys. B*, 1990, **4**, 2217-2268.
17. Conway, J.H. and Sloane, N.J.A. *Sphere Packings, Lattices and Groups*, Springer-Verlag, New York, 1988.
18. Koca, M., Koca, N.O. and Koc, R. 12-Fold symmetric quasicrystallography from higher dimensional lattices. 2013, *arXiv*: 1306.3316v2.
19. Geim, A.K. and Novosolev, K.S. The rise of graphene. *Nat. Mat.*, 2007, **6(3)**, 183-191.
20. Hamilton, S.W.R. *Lectures on Quaternions* London: Whittaker, 1853.
21. Koca, M., Koc, R., Al-Barwani, M. Noncrystallographic Coxeter group H4 in E8. *J. Phys. A: Math. Gen. A*, 2001, **34**, 11201-11213.
22. Conway, J.H. and Smith, D.A. *On Quaternions and Octonions: Their Geometry, Arithmetics, and Symmetry* A.K. Peters, Ltd. Natick, M.A., 2003.
23. Koca, M., Koca, N.O. and Al-Shueili, M. Chiral polyhedra derived from coxeter diagrams and quaternions. *SQU J. for Sci.*, 2011, **16**, 82-101.
24. Ashcroft, N.W. and Mermin, N.D. *Solid State Physics*, W.B. Saunders Company, 1976.

Received 20 October 2013
Accepted 9 December 2013